A Technique for Developing an Entropy Consistent System of Second-Order Hydrodynamic Equations

Ramesh Balakrishnan[†] and Ramesh K. Agarwal[††]

[†]Center for Simulation of Advanced Rockets, University of Illinois at Urbana-Champaign, Urbana, IL 61801
[††]National Institute for Aviation Research, Wichita State University, Wichita, KS 67260

Abstract. This paper presents the development of a novel set of second-order hydrodynamic equations known as the BGK-Burnett equations for computing flows in the continuum-transition regime. The second-order distribution function that forms the basis of this formulation is approximated by the first three terms of the Chapman-Enskog expansion. Such and expression, however, does not readily satisfy the moment closure property. Hence an exact closed form expression for the same is obtained by enforcing moment closure and solving a system of algebraic equations to determine the closure coefficients. Through a series of conjectures the closure coefficients are designed to move the resulting system of hydrodynamic equations towards an entropy consistent set. An important step in the formulation of the higher-order distribution functions is the proper representation of the material derivatives in terms of the spatial derivatives. While the material derivatives in the first-order distribution function are approximated by the Euler equations, proper representations to these derivatives in the second-order distribution function are determined by an entropy consistent relaxation technique. The BGK-Burnett equations, obtained by taking moments of the Boltzmann equation in the second-order distribution function, are shown to be stable to small wavelength disturbances and entropy consistent for a wide range of grid points and Mach numbers.

The Need for Higher-Order Hydrodynamic Equations

Orbital Transfer Vehicles (OTVs) belong to a class of hypersonic vehicles that are required to return to a low earth orbit from a high earth orbit as part of their mission. Consequently, they have a substantial portion of their flight envelope in the continuum-transition regime which lies between the continuum and free molecular regimes. In this regime the drag and aerodynamic heating are very sensitive to the degree of rarefaction and their prediction has posed quite a challenge to designers who have had to resort to empirical correlations based on sparse experimental data. Since the ability to conduct ground based experiments to acquire data is a prohibitively expensive option, it would be highly desirable to have a computational technique which can provide data that compares favorably with flow measurements from the Space Shuttle. Such a technique may then be used to predict the hypersonic flowfield for future applications.

In the continuum-transition flow regime, also known as the transitional flow regime, the Knudsen number ($Kn = \lambda/L_{ref}$ where λ denotes the mean fee path and L_{ref} denotes the reference length) is in the neighborhood of unity. In this regime the Navier-Stokes equations yield inaccurate results, as the approximations made in the constitutive relations for the stress and heat flux terms, while acceptable in the continuum regime, are not appropriate in the transitional regime. The insufficient number of collisions between the molecules prevents the gas from attaining thermodynamic equilibrium. This gives rise to regions of non-equilibrium where more general constitutive relations are required to model the flow. To complicate matters even further, there may be regions of continuum and rarefaction that occur side by side. For instance, in the flow field around the OTVs when they re-enter the upper atmosphere, the region close to the fore-body can be represented as a continuum, while the wake region exhibits a high degree of rarefaction.

Currently the only viable technique for computing flows in this regime is the Direct Simulation Monte Carlo (DSMC), although the large number of molecules required for meaningful results makes this method prohibitive with regard to computational time and storage requirements. Hence, there is a need for an extended set of governing equations which incorporates more general expressions for the constitutive relations. On including these constitutive relations in traditional CFD solvers (Navier-Stokes solvers in the continuum domain) it is expected that in addition to capturing the intricacies of the flow field they will also prove to be computationally faster than Monte Carlo simulations.

REPORT DOCUMENTATION PAGE

Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing this collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE 9 Jul 2000	3. REPORT TYPE AND DATES COVERED

4. TITLE AND SUBTITLE

A Technique for Developing an Entropy Consistent System of Second-Order Hydrodynamic Equations

5. FUNDING NUMBERS

6. AUTHOR(S)

Ramesh Balakrishnan and Ramesh K. Agarwal

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

University of Illinois at Urbana-
Champaign, Urbana,
Center for Simulation of Advanced
Rockets,
Urbana, Ill.

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)

10. SPONSORING / MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION / AVAILABILITY STATEMENT

Approved for Public Release; Distribution is unlimited

12b. DISTRIBUTION CODE

A

13. ABSTRACT (Maximum 200 Words)

14. SUBJECT TERMS

15. NUMBER OF PAGES

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT

NSN 7540-01-280-5500

Standard Form 298 (Rev. 2-89)
Prescribed by ANSI Std. Z39-18
298-102

The formulation of a system of second-order hydrodynamic equations relies on the fact that these equations can be obtained by taking moments of the Boltzmann equation, in the second-order distribution function, with the collision invariant vector. In an attempt to derive an expression for the second-order stress, Burnett [1] developed a method by which corrections to the distribution function could be calculated to any degree of approximation. This development considered a general force law between molecules which varied inversely as the nth power of their distance. In a subsequent paper, Burnett [2] derived the complete expression for the second-order distribution function for two extreme cases: (a) Maxwellian molecules, for which the force law varies inversely as the fifth power of the distance and (b) molecules which are modeled as elastic spheres.

In their first successful attempt at computing hypersonic flows using a second-order set of governing equations, Fiscko and Chapman [3] extended the numerical methods for continuum flow into the continuum-transition regime by incorporating the Burnett expressions for stress and heat flux into standard Navier-Stokes solvers. They solved the hypersonic shock structure problem by relaxing an initial solution to steady state and obtained solutions for a monatomic hard sphere gas and argon. Their solutions, obtained on coarse grids for a wide range of Mach numbers, showed that the Burnett solutions were in close agreement with Monte-Carlo simulations and experimental measurements (see Alsmeyer [4]). However, grid refinement studies indicated that the equations became unstable as the mesh size was made progressively finer. This was predicted by Bobylev [5] who showed that the Burnett equations are unstable to small wavelength disturbances.

In an effort to overcome these instabilities, Zhong [6] formulated the *augmented* Burnett equations by adding linear third-order terms from the super-Burnett equations. The coefficients (weights) of these linear third-order terms were determined by a linearized stability analysis of the *augmented* Burnett equations. These equations were successful in computing the hypersonic shock structure and hypersonic blunt body flows. Their initial successes were, however, short lived. Attempts at computing blunt body wakes and flat plate boundary layers with the *augmented* Burnett equations have not been successful. It was observed that these equations could orient the flow in a physically unrealistic manner by allowing shear layers to sharpen to discontinuities and permitting heat flow from cold to hot regions! Since this behavior is in violation of the second-law of thermodynamics it was conjectured that this entropy inconsistency may indeed be the cause of the computational instability. Following this line of thought a rigorous thermodynamic analysis of the Burnett equations ensued, where it was shown by Comeaux [7] that the Burnett equations, when applied to the hypersonic shock structure problem, can violate the second law of thermodynamics as the local Knudsen number increases above a critical limit.

BGK-Burnett Equations: A Novel Second-Order Formulation

While the work of Comeaux [7] demonstrated that the Burnett equations can violate the second-law of thermodynamics, it was still not clear what factors gave rise to negative irreversible entropy. One of the causes for such unphysical effects could arise from the fact that the higher-order hydrodynamic equations do not form a closed set. Also, as mentioned earlier, the Burnett coefficients were derived for Maxwellian and hard sphere gas models. For a real gas, the coefficients were assumed to lie between these two extremes and were determined using an interpolation scheme devised by Lumpkin [8]. Further, it was noticed, by the first author (see Balakrishnan [9]), that although the Burnett equations did take into account the influence of forces between molecules (appropriately modeled) it did not incorporate the corresponding higher-order virial expansion for the equation of state. In all prior attempts at computing the Burnett equations [6, 7], the ideal gas law had been assumed. Another cause for such unphysical effects lies in the improper representation of the material derivatives in the second-order stress and heat flux terms, in terms of the spatial derivatives. Based on these observations, the following objective was drawn up to address the formulation of a novel set of second-order hydrodynamic equations that is designed to be entropy consistent.

■ OBJECTIVE. *In order to understand the dynamics of the process by which the solution evolves in the system of equations obtained from the second-order distribution function, it was decided that the second-order equations be formulated on the same assumptions used to derive the Navier-Stokes equations. While such a formulation does not consider the force of attraction between molecules, a factor that contributes largely to the dynamics of molecular collisions at low pressures, it must be emphasized that a proof of entropy consistency at this fundamental level is necessary before considering all other factors that characterize flows in the continuum-transition regime.*

Boltzmann Equation with the BGK model for the Collision Integral

A molecule is characterized by its position $\mathbf{r}$, velocity $\mathbf{v}$ and internal energy ϵ which together constitutes a 7-dimensional phase space. In kinetic theory, a gas is described by a distribution function which contains information regarding the

distribution of molecules, their velocities and (in the present formulation) their internal energy. The distribution function expresses the probability of finding molecules in the physical volume d^3r whose velocities and internal energy lie in the range $\mathbf{v}$ to $\mathbf{v} + d\mathbf{v}$ and ϵ to $\epsilon + d\epsilon$ respectively. The number density or expected number of such molecules per unit volume (in physical space) is defined as

$$n(\mathbf{r}, t) = \int_{\mathbb{R}^3} \int_{\mathbb{R}^+} \mathscr{F}(t, \mathbf{r}, \mathbf{v}, \epsilon) d^3v d\epsilon \tag{1}$$

where $\mathscr{F} = \mathscr{F}(t, \mathbf{r}, \mathbf{v}, \epsilon) : \mathbb{R}^+ \times \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^+ \to \mathbb{R}^+$ defines the distribution function. The flow variables that are described by the hydrodynamic equations are averages of quantities that depend on the velocity and internal energy of the constituent molecules. These averages are defined as moments of the distribution function.

■ DEFINITION. *The moment of a function, $\phi = \phi(t, \mathbf{v}, \epsilon) : \mathbb{R}^+ \times \mathbb{R}^3 \times \mathbb{R}^+ \to \mathbb{R}$, is defined as the inner product*

$$\langle \phi(t, \mathbf{v}, \epsilon), \mathscr{F}(t, \mathbf{r}, \mathbf{v}, \epsilon) \rangle = \int_{\mathbb{R}^3} \int_{\mathbb{R}^+} \phi(t, \mathbf{v}, \epsilon) \mathscr{F}(t, \mathbf{r}, \mathbf{v}, \epsilon) d^3v d\epsilon, \tag{2}$$

over the molecular space $\Xi = \{(\mathbf{v}, \epsilon) | \mathbf{v} \in \mathbb{R}^3 \text{ and } \epsilon \in \mathbb{R}^+ \}$.
The average of $\phi(t, \mathbf{v}, \epsilon)$ may also be written as

$$\bar{\phi}(\mathbf{r}, t) = \langle \phi(\mathbf{v}, \epsilon), f(t, \mathbf{r}, \mathbf{v}, \epsilon) \rangle = \int_{\mathbb{R}^3} \int_{\mathbb{R}^+} \phi(t, \mathbf{v}, \epsilon) f(t, \mathbf{r}, \mathbf{v}, \epsilon) d^3v d\epsilon, \tag{3}$$

where the normalized distribution function is defined as $f(t, \mathbf{r}, \mathbf{v}, \epsilon) = \dfrac{\mathscr{F}(t, \mathbf{r}, \mathbf{v}, \epsilon)}{n(\mathbf{r}, t)}$.

If the gas is assumed to be composed of a single species of identical molecules, then in the absence of external forces, the equation expressing the conservation of molecules in a fixed spatial domain $\Omega \subset \mathbb{R}^3$ is given by

$$\frac{\partial}{\partial t} \int_{\Omega} n \langle f \rangle \, d\Omega + \int_{\Omega} \nabla_{\mathbf{r}} \cdot (n \langle f \rangle \mathbf{v}) d\Omega = \left[\int_{\Omega} \frac{dn}{dt} d\Omega \right]_{\text{coll}}. \tag{4}$$

On multiplying Eq. (4) throughout by the molecular mass m, we obtain for an infinitesimal volume $\delta\Omega \in \Omega$,

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} \right) \rho f = \left[\frac{d\rho(\mathbf{r}, t)}{dt} \right]_{\text{coll}} = J \left[f(\mathbf{v}, \epsilon), f(\mathbf{v}_1, \epsilon_1) \right]. \tag{5}$$

Owing to the intractable nature of the collision integral, $J \left[f(\mathbf{v}, \epsilon), f(\mathbf{v}_1, \epsilon_1) \right]$, it is approximated by the Bhatnagar-Gross-Krook (BGK) model

$$J[f(\mathbf{v}, \epsilon), f(\mathbf{v}_1, \epsilon_1)] = \nu(f^{(0)} - f) \tag{6}$$

where ν denotes the collision frequency, the local Maxwellian $f^{(0)} = \rho/I_0 \sqrt{\beta/\pi} e^{-I/I_0} e^{-\beta C_x^2}$, $I = \epsilon + v_x^2/2 + v_y^2/2$, $\beta = 1/(2RT)$, u_x denotes the x-component of the fluid velocity ($\mathbf{u}$), $C_x = v_x - u_x$ is the x-component of the thermal or peculiar velocity ($\mathbf{C}$) and $I_0 = \langle I, f^{(0)} \rangle$ denotes the average internal energy. The variables that are conserved in a collision process are expressed by the collision invariant vector $\mathbf{\Psi} = [1, \mathbf{v}, I + (\mathbf{v} \cdot \mathbf{v})/2]^{\text{T}}$.

Second-Order Distribution Function

The Chapman-Enskog expansion for the second-order distribution function is given by the following perturbative expansion about $f^{(0)}$

$$f = f^{(0)} + \xi f^{(1)} + \xi^2 f^{(2)} + \cdots \tag{7}$$

where the local Knudsen number, ξ, is the perturbation parameter. Substituting Eq. (7) in the non-dimensional form of Eq. (6) and equating like powers of the Knudsen number gives

$$f^{(i)} = -\frac{1}{\xi\nu} \left[\frac{\partial f^{(i-1)}}{\partial t} + v_x \frac{\partial f^{(i-1)}}{\partial x} \right] \tag{8}$$

In formulating higher-order distribution functions one starts with the Maxwellian distribution function $f^{(0)}$ and obtains higher-order terms (iterates) in the distribution function by a process of iterative refinement as expressed in Eq. (8).

Since the Euler, Navier-Stokes and other higher-order hydrodynamic equations must have the same field vector, $\mathbf{Q} = [\rho, \rho\mathbf{u}, \rho e_t]^{\mathrm{T}}$, it follows that all higher-order terms in the distribution function, *i.e.* $f^{(i)} \; \forall i \geq 1$, must satisfy the following moment closure property.

■ MOMENT CLOSURE PROPERTY.

$$\left\langle \boldsymbol{\Psi}, \xi^i f^{(i)} \right\rangle = 0, \forall i \geq 1. \tag{9}$$

This requirement ensures that the continuity equation remains unchanged! The generic expression for the second-order distribution function is given by

$$f = f^{(0)} + \xi f^{(1)} - \frac{\xi}{\nu} \left[\frac{\partial}{\partial t} \left(f^{(1)} \right) + \frac{\partial}{\partial x} \left(u_x f^{(1)} \right) + \frac{\partial}{\partial x} \left(f^{(0)} \widetilde{\phi}^{(1)} \right) \right] \tag{10}$$

where

$$\begin{cases} \widetilde{\phi}^{(1)} &= -\frac{1}{\xi\nu} \left[\widetilde{\mathcal{B}}^{(1)}(I, C_x) \frac{\partial \beta}{\partial x} + \widetilde{\mathcal{B}}^{(2)}(I, C_x) \frac{\partial u_x}{\partial x} \right], \\[2mm] \widetilde{\mathcal{B}}^{(1)}(I, C_x) &= \frac{\theta_1}{\beta} C_x^2 + \theta_2 \frac{I}{\beta I_0} C_x^2 + \theta_3 C_x^4, \\[2mm] \widetilde{\mathcal{B}}^{(2)}(I, C_x) &= \theta_4 \beta C_x^3 + \theta_5 \frac{I}{I_0} C_x + \theta_6 C_x, \end{cases} \tag{11}$$

and the moment closure coefficients satisfying the moment closure relation $\left\langle \boldsymbol{\Psi}, f^{(0)} \widetilde{\phi}^{(1)}(I, C_x) \right\rangle = 0$ are given by the expressions

$\omega_1 = \dfrac{97\gamma - 135}{4(9 - 7\gamma)}$	$\omega_2 = -\dfrac{23\gamma - 27}{2(9 - 7\gamma)}$	$\breve{\omega}_1 = \dfrac{17\gamma - 27}{2(9 - 7\gamma)}$	$\omega_3 = -\dfrac{2}{3}(3 - \gamma)$

and

$\theta_1 = \dfrac{5}{2} + \omega_1$	$\theta_2 = \omega_2 - 1$	$\theta_3 = -(1 + \breve{\omega}_1)$
$\theta_4 = (3 - \gamma) + \omega_3$	$\theta_5 = -(\gamma - 1) - \omega_3$	$\theta_6 = \dfrac{(3\gamma - 5)}{2} + \omega_3$

It must be noted that there is no unique way of satisfying the requirement of moment closure. This introduces a certain arbitrariness in the formulation of the second-order distribution function and gives rise to a family of BGK-Burnett equations. Since not all such formulations satisfy the twin requirements of stability and entropy consistency, some additional constraints are required to design the closure coefficients such that the resulting set of equations are entropy consistent and stable. The first author, in his doctoral dissertation has described the formulation and properties of the BGK-Burnett (1996), BGK-Burnett (1998) and BGK-Burnett (1999) equations. The closure coefficients given in this paper are for the BGK-Burnett (1999) equations. In the formulation of the BGK-Burnett (1999) equations the additional constraint that was imposed required that the linearized stability plot (see Bobylev [5] and Balakrishnan [9]) of the BGK-Burnett and N-S equations show similar variations of the roots of the characteristic equation.

Moments of the Boltzmann Equation

A mathematical link between the Boltzmann equation at the kinetic level and the hydrodynamic equations at the fluid level is established by taking *moments* of the Boltzmann equation. It can be shown that moments of the Boltzmann equation with the Maxwellian distribution function give rise to the Euler equations. Likewise, moments of the Boltzmann equation with the first-order distribution function give rise to the Navier-Stokes equations. On taking moments of the Boltzmann equation in the second-order distribution function, Eq. (10), with the collision invariant vector $\boldsymbol{\Psi}$

$$\frac{\partial}{\partial t} \left\langle \boldsymbol{\Psi}, f^{(0)} + \xi f^{(1)} + \xi^2 f^{(2)} \right\rangle + \frac{\partial}{\partial x} \left\langle v_x \boldsymbol{\Psi}, f^{(0)} + \xi f^{(1)} + \xi^2 f^{(2)} \right\rangle = 0 \tag{12}$$

we get the BGK-Burnett equations

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{G}^i}{\partial x} + \frac{\partial \mathbf{G}^v}{\partial x} + \frac{\partial \mathbf{G}^B}{\partial x} = 0 \tag{13}$$

where the flux vectors are given by

$$
\mathbf{G}^i = \begin{pmatrix} \rho u_x \\ p + \rho u_x^2 \\ p u_x + \rho u_x e_t \end{pmatrix}, \quad
\mathbf{G}^v = \begin{pmatrix} 0 \\ -\tau_{xx}^v \\ -u_x \tau_{xx}^v + \dot{q}_x^v \end{pmatrix}, \quad
\mathbf{G}^B = \begin{pmatrix} 0 \\ -\tau_{xx}^B \\ -u_x \tau_{xx}^B + \dot{q}_x^B \end{pmatrix}
\tag{14}
$$

The stress and heat flux expressions in the N-S (superscript v) and BGK-Burnett (superscript B) fluxes are given by

$$
\tau_{xx}^v = (3 - \gamma)\frac{p}{\nu}\frac{\partial u_x}{\partial x}, \quad
\dot{q}_x^v = -\frac{\gamma \mathrm{R}}{(\gamma - 1)}\frac{p}{\nu}\frac{\partial T}{\partial x},
\tag{15}
$$

$$
\begin{aligned}
\tau_{xx}^B = & -\frac{1}{\nu^2}\left[\frac{\Omega_1}{\beta}\frac{\mathscr{D}\rho}{\mathscr{D}t}\frac{\partial u_x}{\partial x} + \underbrace{\Omega_1\frac{\rho}{\beta}\frac{\mathscr{D}}{\mathscr{D}t}\left(\frac{\partial u_x}{\partial x}\right)}_{\boxed{I}} - \Omega_1\frac{\rho}{\beta^2}\frac{\mathscr{D}\beta}{\mathscr{D}t}\frac{\partial u_x}{\partial x} + \Omega_1\frac{\rho}{\beta}\left(\frac{\partial u_x}{\partial x}\right)^2 + \frac{\Omega_2}{\beta^3}\frac{\partial \rho}{\partial x}\frac{\partial \beta}{\partial x} \right. \\
& \left. + \Omega_2\frac{\rho}{\beta^3}\frac{\partial^2 \beta}{\partial x^2} - 3\Omega_2\frac{\rho}{\beta^4}\left(\frac{\partial \beta}{\partial x}\right)^2 \right] + \frac{1}{\nu^3}\underbrace{\left[\Omega_1\frac{\rho}{\beta}\frac{\partial u_x}{\partial x}\frac{\mathscr{D}\nu}{\mathscr{D}t} + \Omega_2\frac{\rho}{\beta^3}\frac{\partial \beta}{\partial x}\frac{\partial \nu}{\partial x} \right]}_{\boxed{II}},
\end{aligned}
\tag{16}
$$

$$
\begin{aligned}
\dot{q}_x^B = & \frac{1}{\nu^2}\left[\Omega_1\frac{\rho}{\beta}\frac{\mathscr{D}u_x}{\mathscr{D}t}\frac{\partial u_x}{\partial x} - \frac{\Omega_3}{\beta^3}\frac{\mathscr{D}\rho}{\mathscr{D}t}\frac{\partial \beta}{\partial x} + 3\Omega_3\frac{\rho}{\beta^4}\frac{\mathscr{D}\beta}{\mathscr{D}t}\frac{\partial \beta}{\partial x} - \underbrace{\Omega_3\frac{\rho}{\beta^3}\frac{\mathscr{D}}{\mathscr{D}t}\left(\frac{\partial \beta}{\partial x}\right)}_{\boxed{III}} + (\Omega_2 - \Omega_3)\frac{\rho}{\beta^3}\frac{\partial \beta}{\partial x}\frac{\partial u_x}{\partial x} \right. \\
& \left. + \frac{\Omega_4}{\beta^2}\frac{\partial \rho}{\partial x}\frac{\partial u_x}{\partial x} + \Omega_4\frac{\rho}{\beta^2}\frac{\partial^2 u_x}{\partial x^2} - 2\Omega_4\frac{\rho}{\beta^3}\frac{\partial \beta}{\partial x}\frac{\partial u_x}{\partial x} \right] + \frac{1}{\nu^3}\underbrace{\left[\Omega_3\frac{\rho}{\beta^3}\frac{\partial \beta}{\partial x}\frac{\mathscr{D}\nu}{\mathscr{D}t} - \Omega_4\frac{\rho}{\beta^2}\frac{\partial u_x}{\partial x}\frac{\partial \nu}{\partial x} \right]}_{\boxed{IV}}.
\end{aligned}
\tag{17}
$$

The presence of the material derivatives ($\mathscr{D}/\mathscr{D}t = \partial/\partial t + u_i\partial/\partial x_i$) in Eqs. (16) and (17) make them the most general expressions for the BGK-Burnett stress and heat flux, and give rise to a large number of representational forms depending on the approximations used to express these derivatives in terms of spatial derivatives. The material derivatives $\mathscr{D}\beta/\mathscr{D}t$ and $\mathscr{D}u_x/\mathscr{D}t$ are approximated by the Euler equations. The representation of terms $\boxed{I}$ and $\boxed{III}$ is determined by an entropy consistent relaxation technique. The inclusion of the derivatives of the collision frequency (ν), in terms $\boxed{II}$ and $\boxed{IV}$, in the formulation of the BGK-Burnett (1998) and BGK-Burnett (1999) equations marks an important step in the derivation. Neglecting these terms in the formulation of the BGK-Burnett (1996) equations yielded expressions for the stress and heat flux that had the *same* derivatives as the Burnett equations. Such an omission, however, leads to the creation of a fictitious viscosity that varies as a function of pressure, as opposed to the temperature, thereby causing a viscous imbalance between the N-S and BGK-Burnett flux vectors that made the equations stiff.

The Entropy Consistent Relaxation Technique and Shock Structure Computations

While it is possible to treat the shock as a sharp discontinuity and use the Euler equations to predict the macroscopic properties of the shock field, the structure of the shock *per se*, in dilute gases, can be only be determined by solving the Boltzmann equation. It has been shown by Liepmann *et. al* [10] that the shock structure in a monatomic perfect gas is contained in the Boltzmann equation. Since the BGK-Burnett equations are formulated to model the gas in a state of collisional and thermodynamic non-equilibrium, it was decided to solve the shock structure problem, as it presents the unique possibilities of (a) studying the behavior of the BGK-Burnett equations by isolating the effects of boundary conditions and (b) arriving at an entropy consistent approximation for the material derivatives in τ_{xx}^B and $\dot{q}_x^B$.

The Navier-Stokes solution to the shock structure problem results in a smooth variation of the flow variables about the discontinuity such that flux equilibrium is restored at all points in the flowfield. Since the Euler and Navier-Stokes equations are known to be entropy consistent, the resulting shock profile does not contain any physical anomalies. However, for the BGK-Burnett equations, the equilibrium requirement may be met by a multitude of of shock shapes, that may

include "physically untenable" solutions. A more meaningful outcome can be expected by insisting that the governing equations satisfy the second-law of thermodynamics at every stage of the solution process where the flow evolves from a given initial profile. Since there are a wide variety of approximations to the material derivatives in the BGK-Burnett fluxes, one must identify a correct approximation that accounts for the differences in time scales between the first- and second-order fluxes and also ensures entropy consistency. In order to determine a proper approximation for the material derivatives, an entropy consistent relaxation technique (ECRT) has been developed (see Balakrishnan [9]), which is based on the following premise:

■ PREMISE. *By considering the Navier-Stokes solution to be an entropy consistent intermediate solution of the BGK-Burnett equation it is possible to select approximations to the material derivatives in τ_{xx}^B and $\dot{q}_x^B$ which will preserve the positivity of the irreversible entropy as the BGK-Burnett solution evolves.*

This above premise is based on the observation that on a relatively coarse mesh, where the local Knudsen number is quite low, the BGK-Burnett solutions are indistinguishable from the Navier-Stokes solution. Further, by considering the BGK-Burnett solution as a second-order relaxation of the Navier-Stokes solution it is entirely justifiable that the Navier-Stokes solution would have developed as an intermediate solution of the BGK-Burnett equations had the latter been started on the initial profile provided by the Rankine-Hugoniot (R-H) relations. Also, tacit in this assumption is the restriction that the BGK-Burnett equations shall at no time during the solution process violate the second-law of thermodynamics. The first step in formulating the ECRT is to develop an expression for the irreversible entropy produced by the BGK-Burnett equation. An expression for this, based on the Boltzmann H-theorem is given by (see Balakrishnan [9])

$$
\dot{\sigma} = \mu R \left[E_1^{(1)} \frac{1}{T^2} \left(\frac{\partial T}{\partial x} \right)^2 + E_2^{(1)} \frac{1}{RT} \left(\frac{\partial u_x}{\partial x} \right)^2 \right] + \frac{\mu^2 R}{p^2} \left[E_1^{(2)} R \frac{\rho}{T} \frac{\partial T}{\partial x} \frac{\mathscr{D}}{\mathscr{D} t} \left(\frac{\partial T}{\partial x} \right) \right.
$$
$$
+ E_2^{(2)} R \frac{\rho}{T} \frac{\partial u_x}{\partial x} \left(\frac{\partial T}{\partial x} \right)^2 + E_3^{(2)} \rho \left(\frac{\partial u_x}{\partial x} \right)^3 + E_4^{(2)} \rho \left(\frac{\partial u_x}{\partial x} \right) \frac{\mathscr{D}}{\mathscr{D} t} \left(\frac{\partial u_x}{\partial x} \right)
$$
$$
\left. + E_5^{(2)} R \rho \frac{\partial T}{\partial x} \frac{\partial^2 u_x}{\partial x^2} + E_6^{(2)} R \rho \frac{\partial u_x}{\partial x} \frac{\partial^2 T}{\partial x^2} + E_7^{(2)} R \frac{\partial \rho}{\partial x} \frac{\partial u_x}{\partial x} \frac{\partial T}{\partial x} \right]. \tag{18}
$$

where terms of $\mathcal{O}(\mu)$ account for the $\dot{\sigma}$ generated by the N-S terms and terms of $\mathcal{O}(\mu^2)$ represent the contribution of the second-order (BGK-Burnett) terms. The $E_j^{(i)}$ coefficients are given in [9]. The essence of the ECRT may now be summarized in the following question:

■ QUESTION. *When viewed as an intermediate solution of the BGK-Burnett equations, what approximation or approximations of the material derivatives in τ_{xx}^B and $\dot{q}_x^B$ would yield an entropy consistent Navier-Stokes distribution ?*

The ECRT, which answers the above question, is applied in the following manner: For a given free stream Mach number the shock structure is computed by solving the Navier-Stokes equations in the given control volume based on the initial conditions specified by the R-H relations. Since the N-S solution may be considered to be an entropy consistent intermediate solution of the BGK-Burnett equations it is imperative that this solution generates a positive $\dot{\sigma}$ as given by Eq. (18). In order to calculate $\dot{\sigma}$ the various approximations for the material derivatives identified by the linearized stability analysis (see Balakrishnan [9]) are substituted in Eq. (18) and checked for positivity. On identifying such an approximation for the material derivative, the same approximation is substituted in the second-order expressions for the stress and heat flux, Eqs. (16-17) and the BGK-Burnett solution proceeds with the N-S solution as the initial condition. Based on the ECRT it was identified that the Navier-Stokes approximation for $\mathscr{D}/\mathscr{D} t \, (\partial u_x/\partial x)$ and setting $\mathscr{D}/\mathscr{D} t \, (\partial T/\partial x) = 0$ give rise to entropy consistent expressions for the second-order stress and heat flux. Figures 1(a)-1(f) show the solutions obtained for the Mach 5 and Mach 20 normal shock for monatomic argon gas. From the solutions it is clear that the differences between the N-S and BGK-Burnett solutions become more pronounced as the free stream Mach number increases. The same is observed in Tables (1) and (2) where the inverse shock thickness (λ_1/t) based on the density, temperature and stress gradients are presented for the Navier-Stokes and BGK-Burnett (1999) solutions.

Blunt Body Flow Computations

In order to consider practical applications, a system of 2-D BGK-Burnett equations was derived by extending the entropy consistent approximations identified in the 1-D formulation. The 2-D BGK-Burnett equations were solved on a coarse (57 × 81) grid for the hypersonic flow past a blunt body for flow conditions representative of moderately high Knudsen numbers. The results of these computations for a free stream Mach number $M_\infty = 10$ at an altitude of 75 km are shown in Figures 1(g)-1(l). These flow conditions correspond to a free stream Knudsen number $Kn_\infty = 0.1$ for a cylinder of radius

Upstream Mach Number	Inverse Density Thickness	Inverse Temperature Thickness	Inverse Stress Thickness
1.2	6.306×10^{-2}	6.211×10^{-2}	4.825×10^{-2}
5.0	0.576815	0.471664	0.308457
10.0	0.647143	0.526993	0.436082
20.0	0.667823	0.542892	0.439383

Table 1: Shock thickness for argon computed using the Navier-Stokes equations. Fine grid solutions, $\Delta x/\lambda_1 = 0.1$.

Upstream Mach Number	Inverse Density Thickness	Inverse Temperature Thickness	Inverse Stress Thickness
1.2	6.20585×10^{-2}	6.18614×10^{-2}	9.21306×10^{-3}
5.0	0.503101	0.375218	0.184188
10.0	0.570015	0.405715	0.307753
20.0	0.586499	0.413692	0.308121

Table 2: Shock thickness for argon computed using the BGK-Burnett (1999) equations. Fine grid solutions, $\Delta x/\lambda_1 = 0.1$.

Rb = 0.02m. It is seen that there are differences in the solutions obtained from the Navier-Stokes and BGK-Burnett (1999) in the region upstream of the bow shock.

Conclusions

A technique to develop a 1-D entropy consistent set of second-order hydrodynamic equations has been presented. These equations, termed the BGK-Burnett equations have been shown to yield thicker shocks when compared to the N-S solutions and are entropy consistent for the range of Mach numbers and grid densities considered in this study. The identification of the fictitious viscosity arising as a result of neglecting the derivatives of ν represents an important step in the formulation of an entropy consistent set of equations. This formulation which is based on the assumption that there is no intermolecular force between molecules needs to be extended to include molecular forces that vary as a function of the intermolecular distances. It is also shown that a direct extension of this formulation to 2-D gives rise to thicker shocks for flows past blunt bodies. However, it remains to be seen if an extension of this methodology to higher dimensions results in entropy consistent formulations.

References

[1] D. Burnett, Proceedings of the London Mathematical Society 385 (1935).

[2] D. Burnett, Proceedings of the London Mathematical Society 382 (1936).

[3] K. A. Fiscko and D. R. Chapman, in *16th International Symposium of Rarefied Gas Dynamics* (Academic Press, New York, 1988).

[4] H. Alsmeyer, Journal of Fluid Mechanics **74**, 497 (1976).

[5] A. V. Bobylev, Sov. Phys. Dokl. **27(1):29**, (1982).

[6] X. Zhong, Ph.D. thesis, Stanford University, 1991.

[7] K. A. Comeaux, Ph.D. thesis, Stanford University, 1995.

[8] F. E. Lumpkin, Ph.D. thesis, Stanford University, 1990.

[9] R. Balakrishnan, Ph.D. thesis, Wichita State University, 1999.

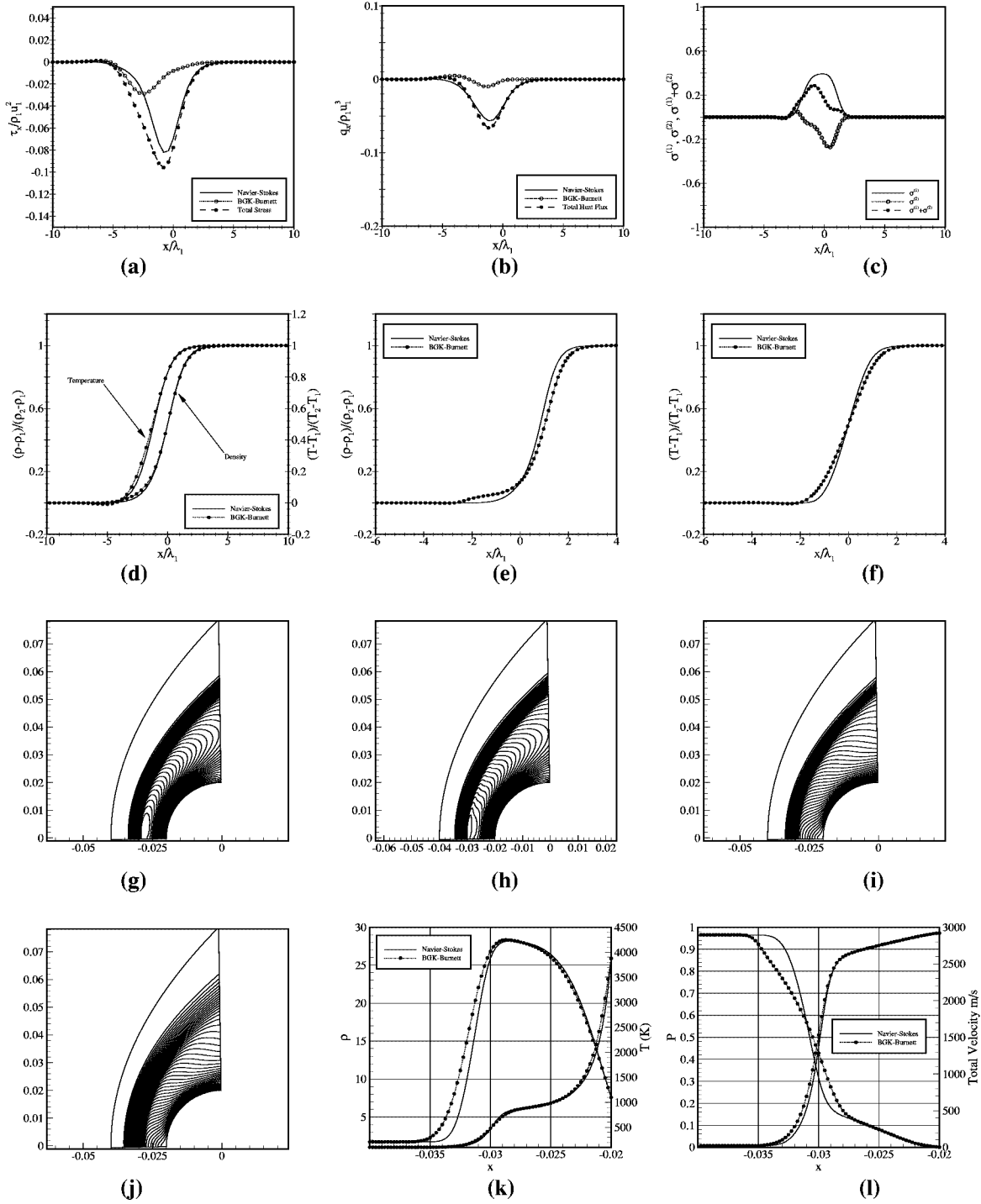[10] H. W. Liepmann, R. Narasimha, and M. T. Chahine, The Physics of Fluids **5**, 1314 (1962).

Figure 1: Figures (a), (b), and (c) show the variations of the stress, heat flux and irreversible entropy due to the Navier-Stokes, and BGK-Burnett fluxes and their total contribution across a Mach 5 normal shock. Figure (d) shows the temperature and density variations across a Mach 5 normal shock while figures (e) and (f) show the same variations across a Mach 20 normal shock. Figures (g) and (h) show the temperature contours for the Navier-Stokes and BGK-Burnett equations respectively while figures (i) and (j) show the velocity contours for the Navier-Stokes and BGK-Burnett equations. Figures (k) and (l) show the variations of the flow properties along the stagnation streamline.